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Professor Otsuka

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Research on Nucleation of II-VI/III-V Semiconductor Heterojunctions
Principal Investigators: R. L. Gunshor and N. Otsuka

Two studies were carried out in this program. The first one is molecular dynamics (MD) simulations of MBE growth of ZnSe, and the second one is the analysis of phase separation of ZnSe based alloy epilayers.

One study involved molecular dynamics simulations based on the Lennard-Jones-Axilrod-Teller (LJAT) potential model [1]. Using a set of interatomic potentials based on thermodynamic data and crystal structure data, the atomic configurations in the (110) surface of ZnSe was simulated and compared with experimentally observed surface structure [2]. Excellent agreement was obtained between experimental and calculated parameters. The atomic configuration in the Se-terminated (100) surface was also simulated. The simulations yielded a (2x1) dimer structure, agreeing with the observations, but at present no experimental data are available for quantitative examinations. The result of the study suggested that these interatomic potential models of ZnSe can be used for MD studies of elementary processes of homoepitaxial growth of ZnSe by MBE.

At the next stage of this MD simulation study, we tried to develop the interatomic potentials of Ga_2Se_3 and Zn_3As_2 in order to investigate the nucleation process of ZnSe on (100)GaAs. It was concluded that the LJAT potential model is too simple to describe those compound structures.

The second part of the program involved an investigation of phase separation in $ZnSe_{1-x}S_x$ and $Zn_{1-y}Mg_ySe_{1-x}S_x$ epilayers. During the course of the transmission electron microscope (TEM) analysis of laser structures grown by MBE, we observed phase separation in a number of ternary and quaternary layers [3]. The phase separation occurred nearly along the [011] direction in the (100) epilayers. All observed quaternary epilayers with sulfur concentrations greater than x=0.2 exhibited strong phase separation. About one half of the $ZnSe_{1-x}S_x$ layers were found to have phase separation. The X-ray microanalysis has shown that the phase separation is described as the formation of S-rich and S-deficient bands.

The only report of experimental studies of the $ZnSe_{1-x}S_x$ system suggests that this alloy is completely miscible at 900°C. We have examined if this observed phase separation can occur under the equilibrium condition by using the delta lattice parameter (DLP) model. According to this model, the $ZnSe_{1-x}S_x$ system is expected to be completely miscible at the temperatures used in the MBE growth, suggesting that the observed phase separation, i.e., compositional modulation, is a kinetically driven phenomenon. The observation that TEM images of $[01\bar{1}]$ cross-sectional samples of epilayers having phase separation exhibit a wavy surface structure, and also that the period of the wavy suface structure exactly matches that of the compositional modulation, suggests a possible mechanism for the compositional modulation as each valley matches a sulfur-rich band. Sulfur the lowest sticking coefficient of any specie and, hence, is likely to attach more efficiently to step or kink sites during the MBE growth. The wavy surface structure results in a periodic variation of the step density; the step density decreases at the hill and increases at the valley region. The wavy surface structure, therefore, may result in a nonuniform incorporation of sulfur atoms and, hence, lead to the compositional modulation.

[1] J.F. Egler, MS. Thesis, Purdue University, December (1993).

[2] C.B. Duke, A. Paton, A. Kahn, and D.W. Tu, J. Vac. Sci. Technol. B2, 366 (1984).

[3] G.C. Hua, N. Otsuka, D.C. Grillo, J. Han, L. He, and R.L. Gunshor, J. Cryst. Growth, 138, 367 (1994).

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